Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Material

High throughput screening of pure silica zeolites for CF_4 capture from electronics industry

Xiao-Dong Li,*[1]

[1]*College of Science, Henan University of Technology, Zhengzhou 450001, China*

The supporting information provides additional details on the experimental results and data analysis of adsorbing and separating CF4 and N2 mixed gases in pure silica zeolites. Specifically, it includes six figures and two tables, which are intended to enhance the reader's understanding of the main paper by providing visual aids and further clarifying the data.

*To whom correspondence should be addressed. E-mail: xiaodongli@haut.edu.cn

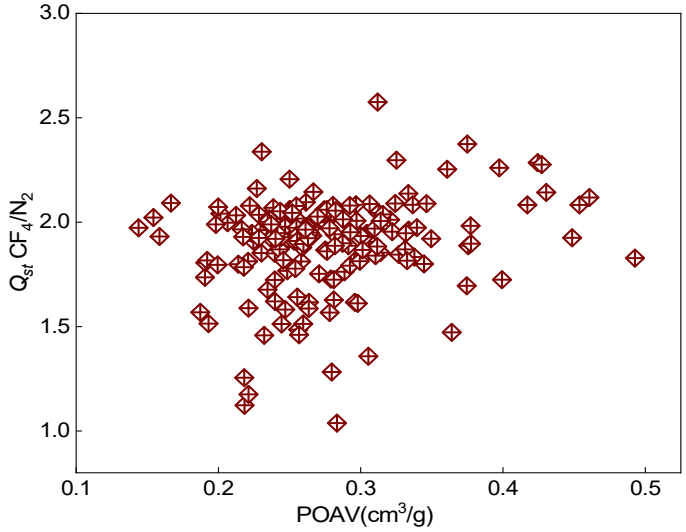

Figure S1. Relationship between the ratio of adsorption heat of CF_4 and N_2 and the pore volume of each zeolite.

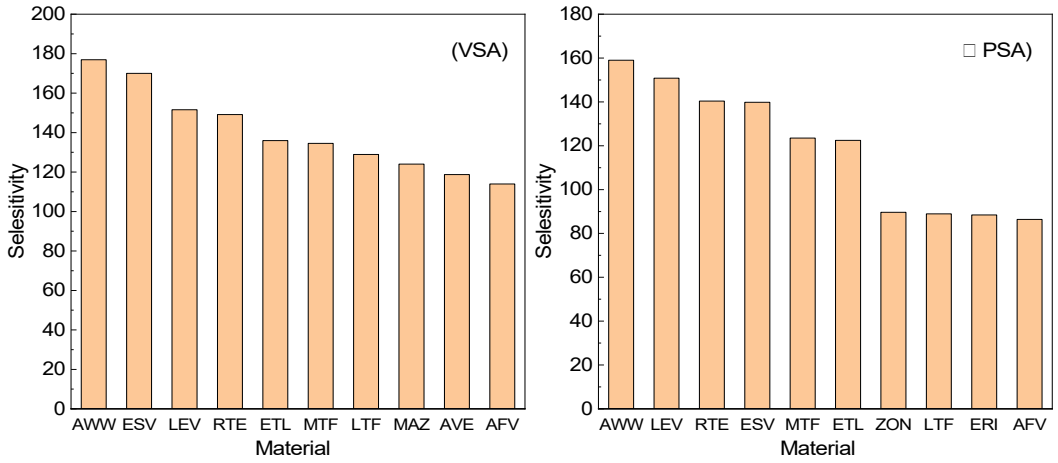

Figure S2. Top ten pure silica zeolite materials ranked by adsorption selectivity (CF_4/N_2) in VSA and PSA processes respectively.

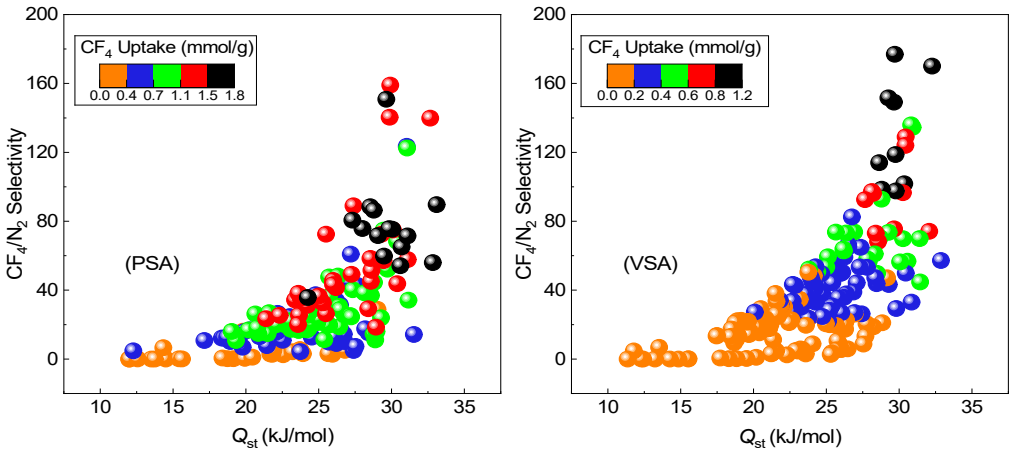

Figure S3. Relationship between the adsorption heat and selectivity of CF_4 on 181 pure silica zeolite structures under VSA and PSA processes, color-mapped by the numerical values of CF_4 adsorption.

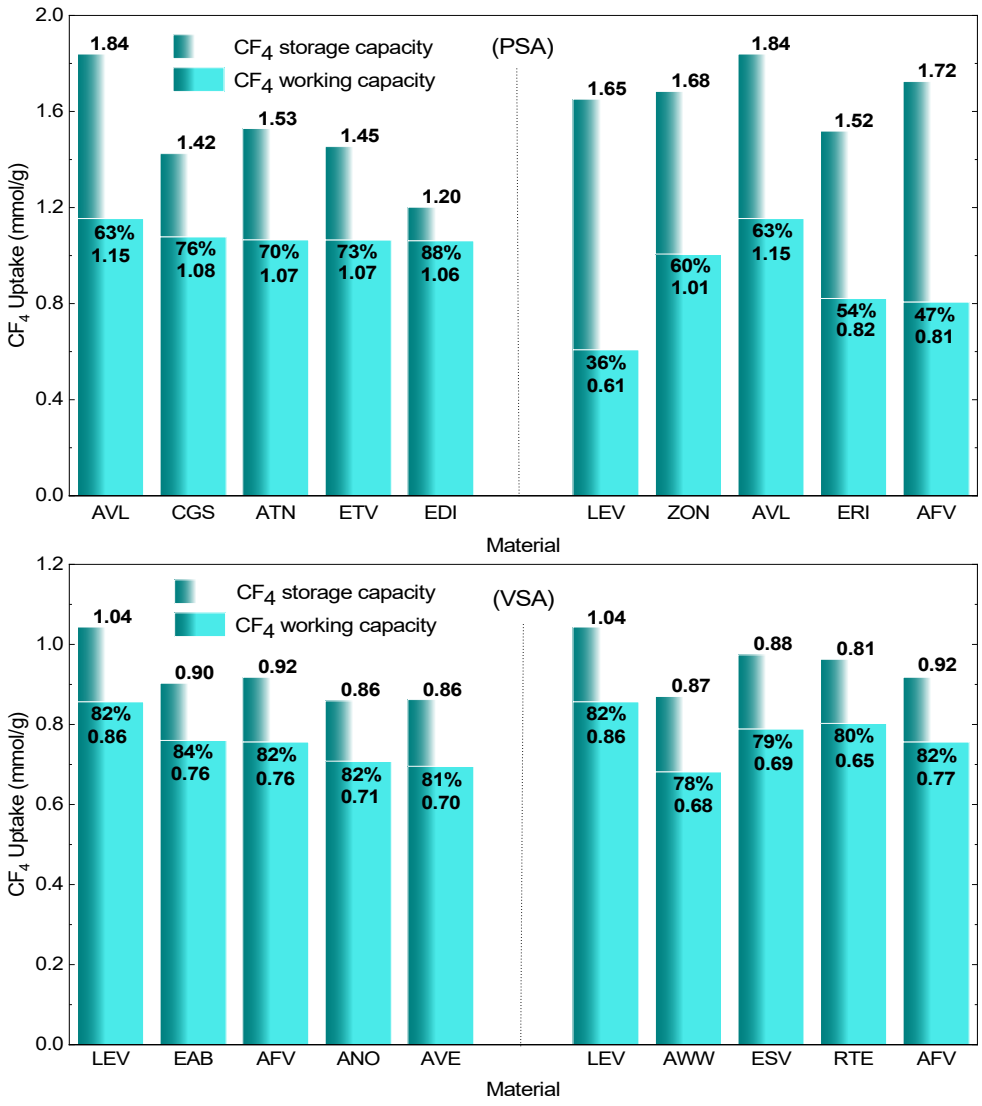

Figure S4. Adsorption capacities of the top five zeolite materials, based on both working capacity and APS, were shown in VSA and PSA processes. The blue area specifically highlights their regenerability.

In the PSA process, the top five zeolite materials in terms of working capacity are AVL, CGS, ATN, ETV, and EDI, while the top five zeolite materials in terms of APS are LEV, ZON, AVL, ERI, and AFV. AVL ranks in the top five for both working capacity and APS, indicating that this material exhibits excellent performance. In the VSA process, the top five zeolite materials in terms of working capacity are LEV, EAB, AFV, ANO, and AVE, while the top five zeolite materials in terms of APS are LEV,

AWW, ESV, RTE, and AFV. Notably, both LEV and AFV appeared in the top five for both work capacity and APS, highlighting their exceptional adsorption and separation performance. In both PSA and VSA processes, EDI and EAB demonstrate the highest regenerability, reaching 88% and 84%, respectively. However, despite EDI's excellent regenerability, its selectivity is only 18.48, resulting in relatively poor adsorption and separation performance for CF_4. In contrast, EAB exhibits a selectivity of up to 97.56, demonstrating excellent adsorption and separation performance for CF_4 compared to most zeolite materials. These findings provide important insights for further understanding and applying these zeolite materials

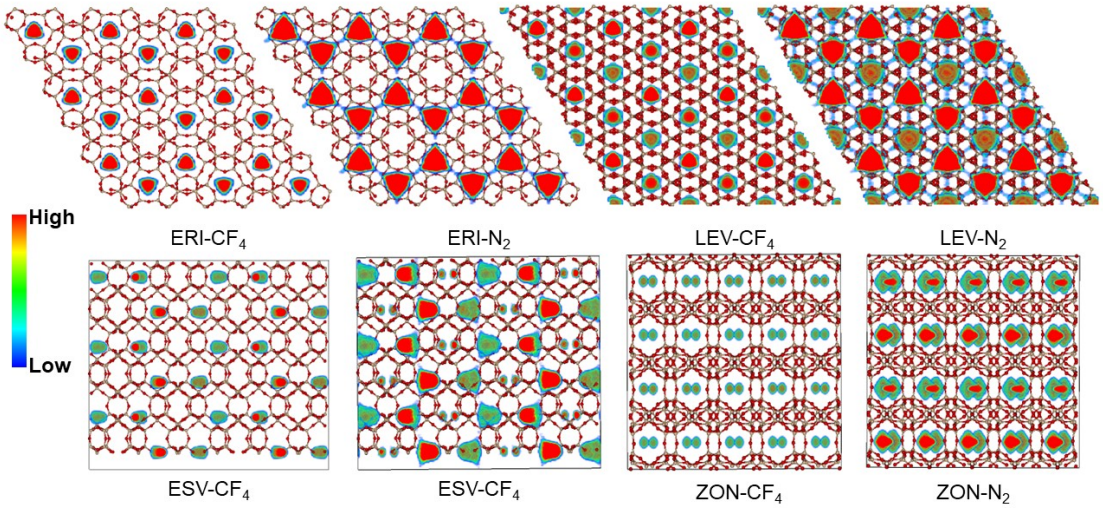

Figure S5. Selected high-performance pure silica zeolite materials ERI, LEV, ESV, and ZON were studied for their preferential adsorption sites for CF_4 and N_2 molecules at 298 K and 1 bar.

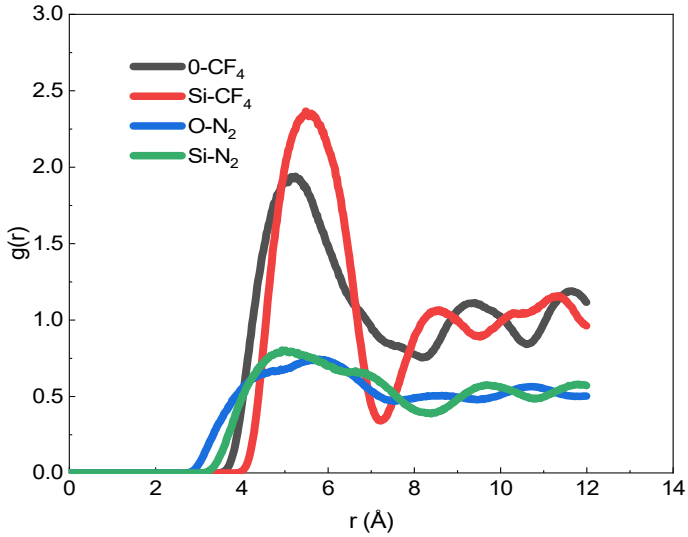

Figure S6. RDF plots of CF_4 and N_2 molecules generated during adsorption and separation of zeolite material AWW at 1 bar and 298 K.

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Table S1. Pore structure parameters of 181 screened pure silica zeolites.

Material	Density (g/cm^3)	LCD (Å)	ASA (m^2/g)	POAV (cm^3/g)	Porosity
AEI	1.50	6.90	1248.14	0.33	0.40
AEL	1.91	5.23	459.55	0.19	0.18
AET	1.82	7.77	506.51	0.22	0.24
AFI	1.69	7.57	643.57	0.26	0.28
AFN	1.74	4.75	746.95	0.25	0.24
AFO	1.92	5.03	472.13	0.19	0.19
AFR	1.51	7.82	1107.97	0.33	0.40
AFS	1.71	9.11	1067.57	0.30	0.42
AFT	1.64	6.78	1146.50	0.31	0.39
AFV	1.57	6.44	1124.84	0.31	0.38
AFX	1.60	6.79	1170.76	0.31	0.39
AFY	1.83	7.42	1192.73	0.30	0.45
ANO	1.65	6.31	880.10	0.28	0.32
APD	1.79	4.22	592.36	0.22	0.21
ASV	1.91	4.95	602.89	0.19	0.21
ATN	1.78	5.51	569.71	0.23	0.23
ATO	2.62	5.34	322.77	0.14	0.18
ATS	1.60	6.58	824.26	0.29	0.32
ATT	1.70	4.89	940.12	0.26	0.29
AVE	1.65	6.02	879.17	0.28	0.33
AVL	1.70	6.28	1027.56	0.28	0.36
AWO	1.82	4.49	527.95	0.22	0.18
AWW	1.69	6.86	773.46	0.26	0.31
BEC	1.51	6.24	1129.63	0.33	0.42
BOF	1.82	5.16	702.09	0.22	0.26
BOG	1.60	7.49	972.96	0.30	0.37
BOZ	1.29	8.31	1790.97	0.45	0.45

Material	Density (g/cm^3)	LCD (Å)	ASA (m^2/g)	POAV (cm^3/g)	Porosity
BPH	1.71	9.11	1061.79	0.30	0.42
BSV	1.87	4.76	757.43	0.22	0.22
CAN	1.91	5.76	474.05	0.23	0.28
CDO	1.80	4.73	720.13	0.22	0.24
CFI	1.67	7.07	631.33	0.27	0.28
CGF	1.90	5.04	262.21	0.20	0.20
CGS	1.69	5.30	962.19	0.27	0.29
CHA	1.90	6.74	989.30	0.26	0.40
CON	1.57	6.76	1054.56	0.31	0.39
CSV	1.62	7.13	983.84	0.29	0.38
DAC	1.74	4.78	869.18	0.24	0.28
DDR	2.19	7.03	452.77	0.19	0.29
DFO	1.59	10.89	1080.76	0.32	0.42
DFT	1.77	4.19	704.69	0.24	0.24
DON	1.71	8.18	593.86	0.26	0.28
EAB	1.59	6.51	1055.49	0.30	0.36
EDI	1.62	4.88	1013.99	0.29	0.30
EMT	1.42	11.00	1057.98	0.40	0.49
EON	1.68	7.27	834.43	0.26	0.30
EPI	1.76	4.90	813.05	0.23	0.28
ERI	1.68	6.30	972.29	0.28	0.35
ESV	1.77	5.65	609.44	0.24	0.27
ETL	1.80	5.77	641.92	0.22	0.22
ETR	1.59	9.61	591.35	0.31	0.36
ETV	1.73	5.27	820.04	0.25	0.28
EUO	1.71	6.19	707.13	0.25	0.28
EWO	1.90	4.64	304.11	0.19	0.16
EWS	1.73	5.46	938.83	0.25	0.31
EZT	1.72	5.90	769.66	0.25	0.30
FAU	1.33	10.70	1128.65	0.42	0.49
FER	1.75	5.14	803.82	0.24	0.28
GIS	1.64	4.57	1181.51	0.28	0.30
GME	1.90	7.12	985.20	0.26	0.39
GON	1.89	5.84	464.20	0.21	0.22
HEU	1.75	5.22	846.77	0.24	0.28
IFO	1.72	7.41	697.74	0.25	0.31
IFR	1.71	6.39	812.41	0.25	0.34
IFW	1.58	7.19	960.62	0.30	0.36
IFY	1.76	6.39	746.67	0.24	0.30
IHW	1.84	6.07	617.22	0.21	0.25
IMF	1.74	6.69	768.85	0.24	0.29
IRN	1.53	8.60	839.28	0.32	0.40
IRR	1.71	13.90	974.85	0.36	0.55
ISV	1.50	6.34	1136.36	0.34	0.41
ITE	1.57	7.77	976.01	0.30	0.36
ITG	1.65	6.42	958.26	0.27	0.35
ITH	1.74	6.30	805.04	0.24	0.28
ITR	1.73	5.96	813.25	0.25	0.29
ITT	1.28	12.77	1271.97	0.45	0.51
IWR	1.56	6.90	1065.55	0.31	0.39
IWS	1.48	7.63	1141.92	0.35	0.43
IWV	1.50	8.11	1004.41	0.34	0.40
IWW	1.66	6.53	912.69	0.28	0.34
JOZ	1.63	4.42	979.74	0.28	0.24
JSN	1.78	4.53	732.07	0.23	0.26
JSR	1.23	7.43	1972.83	0.49	0.52
JST	1.43	4.95	1813.42	0.37	0.37

Material	Density (g/cm^3)	LCD (Å)	ASA (m^2/g)	POAV (cm^3/g)	Porosity
JZO	1.32	11.50	1289.80	0.43	0.50
KFI	1.49	10.16	1227.58	0.34	0.39
LAU	1.80	5.47	719.04	0.23	0.26
LEV	1.59	6.39	1049.10	0.30	0.36
LOV	1.68	3.74	955.55	0.27	0.26
LTA	1.41	10.23	1087.66	0.37	0.46
LTF	1.78	7.72	741.07	0.25	0.29
LTL	1.82	9.61	575.56	0.25	0.29
MAZ	1.96	7.55	730.53	0.23	0.31
MEI	1.67	7.66	1080.50	0.31	0.42
MEL	1.73	6.86	771.45	0.25	0.30
MER	1.63	6.25	1067.12	0.28	0.30
MFI	1.84	5.94	704.46	0.21	0.26
MFS	1.74	6.21	762.15	0.24	0.28
MOR	1.69	6.20	808.92	0.26	0.30
MOZ	1.74	9.63	693.84	0.25	0.29
MRT	1.71	5.38	847.21	0.25	0.28
MSE	1.63	6.49	913.60	0.28	0.35
MTF	2.07	5.57	387.26	0.15	0.19
MTT	1.82	5.48	534.81	0.22	0.21
MTW	1.82	5.31	559.27	0.22	0.23
MWF	1.60	10.06	1159.38	0.29	0.33
MWW	2.08	5.73	766.97	0.23	0.37
NES	1.64	6.17	857.80	0.28	0.32
NPO	1.59	4.91	932.32	0.30	0.28
NPT	1.34	5.76	1693.24	0.42	0.41
OBW	1.27	8.86	1833.09	0.46	0.45
OFF	1.75	6.50	931.91	0.27	0.35
OKO	1.75	6.30	800.49	0.24	0.32
OSI	1.77	6.26	511.21	0.23	0.22
OSO	1.74	5.67	1304.89	0.33	0.42
OWE	1.71	5.18	926.36	0.26	0.30
PAU	1.59	10.08	1174.81	0.30	0.34
PCR	1.87	4.73	557.17	0.20	0.22
PHI	1.63	5.00	1115.91	0.28	0.31
PON	1.81	4.50	658.05	0.22	0.22
POR	1.75	5.39	906.58	0.24	0.31
POS	1.55	6.71	1074.79	0.32	0.40
PSI	2.05	5.34	236.47	0.16	0.11
PTO	1.81	4.82	717.96	0.22	0.25
PTY	1.70	4.67	1016.13	0.26	0.32
PUN	1.49	4.98	1518.86	0.34	0.38
PWN	1.56	9.37	1182.44	0.31	0.36
PWO	1.71	4.75	997.02	0.26	0.32
PWW	1.70	4.72	933.94	0.26	0.31
RHO	1.44	10.03	1235.98	0.36	0.43
RSN	1.68	3.75	925.59	0.27	0.24
RTE	1.71	6.36	762.95	0.25	0.31
RTH	1.61	7.63	945.35	0.29	0.36
RWY	0.76	15.04	2830.28	1.00	0.70
SAF	1.90	6.24	452.25	0.20	0.21
SAO	1.42	8.20	1272.48	0.38	0.47
SAS	1.49	8.55	1021.86	0.33	0.39
SAT	2.29	6.17	626.62	0.20	0.32
SAV	1.46	8.22	1288.67	0.35	0.39
SBE	1.37	12.10	1165.22	0.40	0.45
SBN	1.61	4.39	1087.72	0.29	0.29

Material	Density (g/cm^3)	LCD (Å)	ASA (m^2/g)	POAV (cm^3/g)	Porosity
SBS	1.46	10.95	1117.22	0.38	0.46
SBT	1.46	10.40	1117.92	0.38	0.46
SEW	1.70	6.24	880.82	0.26	0.33
SFE	1.69	6.24	707.13	0.26	0.28
SFF	1.78	7.04	748.55	0.24	0.32
SFG	1.76	6.36	633.62	0.23	0.25
SFH	1.65	7.65	723.95	0.28	0.31
SFN	1.65	7.41	720.77	0.28	0.30
SFO	1.51	7.49	1103.25	0.33	0.39
SFS	1.66	6.76	891.31	0.27	0.34
SFW	1.51	6.79	1244.60	0.33	0.39
SIV	1.63	4.62	1153.53	0.28	0.31
SOF	1.64	4.74	1151.97	0.28	0.34
SOR	1.70	6.41	710.41	0.26	0.29
SOS	1.69	4.37	1095.38	0.27	0.26
SOV	1.53	6.53	1103.28	0.32	0.41
SSF	1.74	7.26	694.17	0.26	0.31
SSY	1.68	6.65	705.68	0.26	0.28
STF	1.68	7.22	830.87	0.26	0.34
STI	1.67	5.82	973.18	0.27	0.33
STT	1.69	6.57	858.70	0.26	0.33
STW	1.77	4.91	1041.14	0.26	0.36
SWY	1.60	6.30	1010.70	0.29	0.35
SZR	1.76	5.59	719.46	0.24	0.25
TER	1.70	6.18	862.81	0.25	0.31
THO	1.57	4.47	1115.56	0.31	0.30
TON	1.81	5.04	534.47	0.22	0.21
TSC	1.32	15.87	1171.34	0.43	0.47
TUN	1.76	7.89	766.66	0.24	0.30
UEI	1.74	5.12	633.60	0.24	0.21
UFI	1.52	9.69	1078.14	0.33	0.42
UOS	1.76	5.32	767.61	0.24	0.25
UOV	1.62	6.21	958.81	0.29	0.36
USI	1.59	6.32	1116.85	0.30	0.37
UTL	1.56	8.49	979.16	0.31	0.40
UWY	1.63	8.38	946.95	0.28	0.35
VET	2.01	5.99	409.11	0.17	0.18
VFI	1.57	11.17	766.18	0.34	0.39
YFI	1.64	7.36	908.74	0.28	0.33
ZON	1.80	5.20	686.67	0.23	0.25

Table S2. Adsorption heat, adsorption capacity, and selectivity of selected pure zeolite materials.

Material	CF_4 Q_{st} (kJ/mol)	N_2 Q_{st} (kJ/mol)	CF_4 Uptake (mmol/g)	N_2 Uptake (mmol/g)	S (CF_4/N_2)
AWW	29.70	14.17	0.870	0.044	176.93
ESV	32.27	15.91	0.876	0.046	170.04
LEV	29.26	14.04	1.044	0.062	151.59
RTE	29.64	14.50	0.811	0.049	149.15
MAZ	30.43	13.02	0.690	0.050	124.05
ZON	32.07	16.66	0.677	0.082	74.14
ETR	29.29	11.37	0.403	0.049	73.56
PCR	32.87	16.10	0.358	0.056	57.17
LTA	27.91	11.76	0.582	0.093	56.29
VFI	13.53	7.85	0.025	0.034	6.77
RWY	11.79	6.76	0.046	0.089	4.68
PON	18.31	15.57	0.001	0.059	0.21
AWO	18.84	16.77	0.001	0.050	0.21
JOZ	15.54	14.97	0.001	0.040	0.11